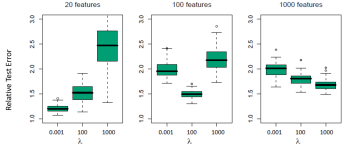
Supervised Learning

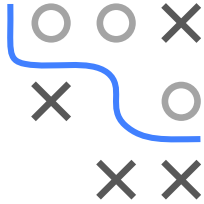
Feature Selection



Learning goals

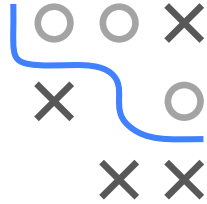
- Understand the practical importance of feature selection.
- Understand that models with integrated selection do not always work.
- Know different types of selection methods.

MOTIVATING EXAMPLE 1: REGULARIZATION

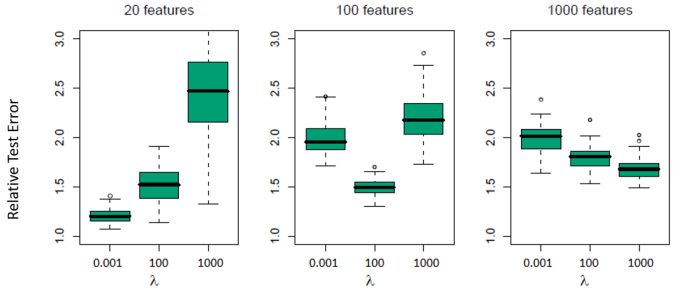


- In case of $p \gg n$, overfitting becomes increasingly problematic.
- This can be demonstrated with a simulation study of three datasets of feature dimensionalities $p \in \{20, 100, 1000\}$ and $n = 100$ samples over 100 simulation runs.
- For each dataset, p features are drawn from a standard Gaussian with pairwise correlation $\rho = 0.2$.
- Target is simulated as $y = \sum_{j=1}^{p} x_j \theta_j + \sigma\varepsilon$, where ε and $\boldsymbol{\theta}$ are both sampled from standard Gaussians, and σ is fixed such that the signal-to-noise ratio is $\text{Var}(\mathbb{E}[y|X])/\sigma^2 = 2$.
- Three ridge regression models with $\lambda \in \{0.001, 100, 1000\}$ are then fitted to each simulated dataset.

MOTIVATING EXAMPLE 1: REGULARIZATION



- Boxplots show the relative test error (RTE $=$ test error$/$Bayes error σ^2) over 100 simulations for the different values of p and λ.

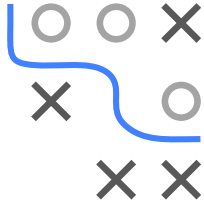


- Lowest RTE is obtained at $\lambda = 0.001$ for $p = 20$, at $\lambda = 100$ for $p = 100$,and at $\lambda = 100$ for $p = 100$.
- Optimal amount of regularization increases monotonically in p here.

$\Rightarrow$ High-dimensional settings require more complexity control through regularization or feature selection.

MOTIVATING EX. 2: COMPARISON OF METHODS

Generalization performance of eight classification methods on micro-array data with $|\mathcal{D}_{\text{train}}| = 144$, $|\mathcal{D}_{\text{test}}| = 54$, $p = 16,063$ genes and a categorical target encoding the type of cancer with 14 classes.

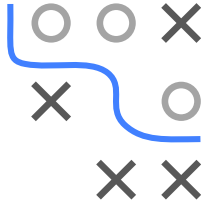


Methods	CV errors (SE) Out of 144	Test errors Out of 54	Number of Genes Used
1. Nearest shrunken centroids	35 (5.0)	17	6,520
2. L_2-penalized discriminant analysis	25 (4.1)	12	16,063
3. Support vector classifier	26 (4.2)	14	16,063
4. Lasso regression (one vs all)	30.7 (1.8)	12.5	1,429
5. k-nearest neighbors	41 (4.6)	26	16,063
6. L_2-penalized multinomial	26 (4.2)	15	16,063
7. L_1-penalized multinomial	17 (2.8)	13	269
8. Elastic-net penalized multinomial	22 (3.7)	11.8	384

Hastie (2009). The Elements of Statistical Learning

Methods without in-built FS do not perform well, with best results obtained using only small subset of relevant features!

MOTIVATING EX. 3: COMPARING FS WITH INTEGRATED SELECTION METHODS



Set-up for simulated micro-array data:

- We simulate micro-array data with function `sim.data` of the package **penalizedSVM**.
- We generate $n = 200$ samples with $p = 100$ features drawn from a MV Gaussian.
- Each simulated sample has $p = 100$ genes, of which half are relevant for the target and half have no influence.
- Among the informative features, 25 are positively and 25 negatively correlated with target.

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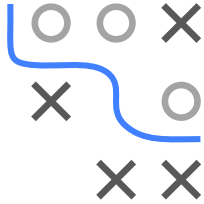

- We compare several classifiers regarding their misclassification rate, of which two have integrated FS (rpart and rForest).
- Since we have few observations, we use repeated 10-fold cross-validation with 10 repetitions.

	rpart	lda	logreg	nBayes	knn7	rForest
all feat.	0.44	0.27	0.25	0.32	0.37	0.36
relevant feat.	0.44	0.18	0.19	0.27	0.33	0.30

$\Rightarrow$ The models with integrated selection do not work ideally here! Also, methods with lin. decision boundary are better due to our simulation set-up.

$\Rightarrow$ Performance improves significantly for most methods when only trained on informative features.